C6 trimer isomer	neat	inf CDCl3	lambda	shift at s= 0.35	^{13}C label	inf C6D6	lambda	shift at s	assignment	ACD/I	ChemDraw
C6-A	135.238	135.034	0.17	135.144075	1-^{13}C	135.429	-0.028	135.35578	C_8	133.75	133.5
	130.248	129.961	0.24	130.11605	2-^{13}C	130.518	-0.015	130.420088	C_9	127.7	129
	43.626	43.178	0.233	43.3878075	1-^{13}C	43.66	0.041	43.6574275	C_6	43.62	43.3
	40.928	40.41	0.245	40.6470375	2-^{13}C	41.031	0.031	41.0020025	C_7 (CH)	43.08	40.6
	38.144	37.733	0.213	37.9253075		38.229	0.102	38.222455	C_4	36.65	37.5
	36.518	36.089	0.226	36.290565		36.625	0.071	36.6037025	C_{15}	34.95	35.5
	32.607	32.258	0.202	32.426105		32.692	0.06	32.6759	C_{10}	32.75	33.7
	32.29	31.94	0.205	32.1091375		32.294	0.096	32.31444	C_{11}	32.17	32.1
	30.331	30.014	0.206	30.171815	2-^{13}C	30.521	0.02	30.45905	C_5 (CH)	30.67	31.1
	29.91	29.544	0.217	29.7214675		30.047	0.059	30.0124725	C_{16}	29.53	29.7
	29.642	29.279	0.204	29.45246		29.729	0.079	29.7165225	C_3	29.17	29.3
	23.318	23.013	0.19	23.162975		23.451	0.092	23.42538	C_{17}	23.06	23.1
	23.133	22.832	0.181	22.9785275		23.29	0.091	23.2557525	C_2	22.93	23
	22.411	22.109	0.189	22.2576975		22.495	0.108	22.49017	C_{12}	22.1	22.8
	19.383	19.253	0.055	19.3110125	1-^{13}C	19.513	-0.033	19.4599925	C_{14}	20.44	21.4
	14.283	14.172	0.049	14.2219975				4.99905	C_1	14.4	14.1
	14.255	14.143	0.059	14.1956225				4.98925	C_{18}	14	14.1
	14.044	13.938	0.061	13.9889775		14.127	0.016	14.10159	C_{13}	13.8	14.2
C6-A'	135.558	135.386	0.173	135.485558	1-^{13}C	135.791	-0.03	135.702625	C_8	133.75	133.5
	130.007	129.71	0.213	129.862408	2-^{13}C	130.241	-0.037	130.150683	C_9	127.7	129
	43.965	43.487	0.227	43.7059425	1-^{13}C	43.987	0.057	43.9922675	C_6	43.62	43.3
	40.781	40.257	0.241	40.4952275	2-^{13}C	40.885	0.023	40.8538325	C_7 (CH)	43.08	40.6
	36.103	35.857	0.22	35.99315		36.265	0.082	36.226955	C_4	36.65	37.5
	35.753	35.254	0.216	35.47779		35.825	0.054	35.812085	C_{15}	34.95	35.5
	32.65	32.294	0.201	32.4643275		32.737	0.062	32.720655	C_{10}	32.75	33.7
	32.325	31.94	0.2	32.12025		32.324	0.09	32.344825	C_{11}	32.17	32.1
	30.267	29.927	0.201	30.0917275	2-^{13}C	30.423	0.02	30.37295	C_5 (CH)	30.67	31.1
	29.823	29.457	0.216	29.63424		29.965	0.06	29.92895	C_{16}	29.53	29.7
	29.436	29.056	0.202	29.234955		29.516	0.086	29.507565	C_3	29.17	29.3
	23.377	23.039	0.177	23.1975675		23.482	0.09	23.465725	C_{17}	23.06	23.1
	23.142	22.85	0.178	22.992695		23.301	0.07	23.261275	C_2	22.93	23
	22.454	22.149	0.186	22.298065		22.536	0.107	22.5316425	C_{12}	22.1	22.8
	20.633	20.422	0.062	20.509955	1-^{13}C	20.737	-0.01	20.698325	C_{14}	20.44	21.4
	14.293	14.18	0.055	14.2320625				5.00255	C_1	14.4	14.2
	14.254	14.147	0.061	14.1983275				4.9889	C_{18}	14	14.1
	14.064	13.938	0.059	13.9955225		14.146	0.016	14.12094	C_{13}	13.8	14.1
C6-B	135.484	135.503	0.178	135.536845	1-^{13}C	135.758	-0.024	135.65664	C_8	138.4	133.5
	129.319	129.097	0.2	129.2202	2-^{13}C	129.56	-0.006	129.474285	C_9	124.6	129
	44.485	43.983	0.217	44.2080675	1-^{13}C	44.484	0.071	44.5005025	C_6	43.62	43.3
	36.563	36.276	0.206	36.423315		36.689	0.085	36.6642375	C_4	36.65	37.5
	36.092	35.586	0.219	35.8129225		36.143	0.069	36.1408475	C_{15}	34.95	35.5
	35.012	34.673	0.215	34.8405625	2-^{13}C	35.177	0.027	35.1253925	C_7 (CH)	43.08	34.6
	32.561	32.19	0.207	32.3669425		32.58	0.086	32.592915	C_{11}	31.95	32.1
	30.627	30.301	0.205	30.4617375	2-^{13}C	30.774	0.021	30.7273275	C_5 (CH)	30.67	31.1
	29.916	29.565	0.221	29.7381275		30.034	0.049	30.0038475	C_{16}	29.53	29.7
	29.668	29.27	0.169	29.4477475		29.727	0.091	29.7270525	C_3	29.17	29.3
	27.87	27.521	0.202	27.689105		28.018	0.021	27.9709775	C_{10}	27.47	27.7
	23.468	23.148	0.19	23.303225		23.602	0.078	23.572845	C_{17}	23.06	23.1
	23.26	22.958	0.188	23.10647		23.406	0.088	23.37492	C_2	22.93	23
	22.807	22.513	0.18	22.65685		22.883	0.057	22.8693675	C_{12}	22.3	22.8
	20.695	20.473	0.064	20.56526	1-^{13}C	20.787	-0.009	20.7527525	C_{14}	20.44	21.4
	14.305	14.192	0.06	14.2452				5.00675	C_1	14.4	14.1
	14.256	14.141	0.064	14.19581				4.9896	C_{18}	14	14.1
	14.145	14.021	0.06	14.07805		14.235	0.006	14.204865	C_{13}	13.9	14.2
C6-B'	135.19	135.181	0.172	135.22328	1-^{13}C	135.444	-0.026	135.349185	C_8	138.4	133.5
	129.674	129.447	0.199	129.571723	2-^{13}C	129.947	-0.009	129.849403	C_9	124.6	129
	44.058	43.596	0.233	43.8107075	1-^{13}C	44.068	0.058	44.077695	C_6	43.62	43.3
	38.146	37.733	0.211	37.9255525		38.225	0.106	38.221465	C_4	36.65	37.5
	36.749	36.315	0.219	36.5167225		36.836	0.092	36.82648	C_{15}	34.95	35.5
	35.145	34.786	0.214	34.960335	2-^{13}C	35.296	0.035	35.2511125	C_7 (CH)	43.08	34.6
	32.599	32.236	0.21	32.410825		32.629	0.087	32.6382925	C_{11}	31.95	32.1
	30.54	30.272	0.211	30.4138025	2-^{13}C	30.72	0.026	30.662915	C_5 (CH)	30.67	31.1
	29.946	29.583	0.218	29.759645		30.052	0.047	30.0255925	C_{16}	29.53	29.7
	29.613	29.258	0.204	29.42866		29.695	0.085	29.6856375	C_3	29.17	29.3
	27.877	27.553	0.204	27.71281		28.039	0.029	27.9888975	C_{10}	27.47	27.7
	23.341	23.033	0.193	23.1847075		23.16	0.075	23.2404125	C_{17}	23.06	23.1
	23.25	22.941	0.186	23.091465		23.397	0.085	23.3648875	C_2	22.93	23
	22.764	22.484	0.18	22.62295		22.843	0.064	22.82991	C_{12}	22.3	22.8
	19.763	19.601	0.067	19.6729425	1-^{13}C	19.901	-0.021	19.8479225	C_{14}	20.44	21.4
	14.281	14.17	0.05	14.220225				4.99835	C_1	14.4	14.2
	14.255	14.135	0.068	14.19247				4.98925	C_{18}	14	14.1
	14.16	14.036	0.058	14.092595		14.239	0.025	14.2170375	C_{13}	13.9	14.1
C6-C	148.142	149.162	0.336	148.88144	2-^{13}C	148.947	-0.025	148.659563	C_5	148.1	155.2
	110.681	109.981	0.034	110.233735	1-^{13}C	110.763	-0.136	110.70336	C_{14}	111.3	107.8
	41.585	41.311	0.199	41.4521725	1-^{13}C	41.72	0.021	41.6775275	C_6	41.83	42.8
	35.682	35.411	0.205	35.5524875		35.845	0.052	35.79978	C_4	35.25	37.3
	35.551	35.224	0.211	35.3864525	2-^{13}C	35.713	0.027	35.6624425	C_7 (CH)	37.25	35.6
	33.798	33.458	0.203	33.6231825	1-^{13}C	33.939	0.038	33.898295	C_8	33.1	33.4
	33.479	33.143	0.207	33.3076925		33.639	0.039	33.5918725	C_{15}	33.1	33.1
	32.325	31.946	0.208	32.12597		32.357	0.159	32.3819725	C_{11}	32.48	31.8
	30.307	29.986	0.204	30.14476		30.372	0.178	30.389745	C_{10}	29.85	29.6
	30.138	29.759	0.207	29.9387425		30.236	0.132	30.23173	C_3	29.65	29.6
	29.14	28.811	0.21	28.973925		29.246	0.053	29.2209575	C_{16}	29	29.6
	26.855	26.522	0.195	26.6829125	2-^{13}C	27	0.047	26.9599425	C_9	27.29	27.5
	23.419	23.123	0.176	23.26664		23.561	0.076	23.52859	C_{17}	23.2	23
	23.043	22.708	0.174	22.864835		23.123	0.107	23.1193425	C_{12}	22.83	22.7

C5 trimer isomer	neat	inf CDCl3	lambda	shift at s=	inf C6D6	lambda	shift at s	assignment	ACD/I	ChemDraw
C5-A	135.43	135.1934	0.1529	135.310995	135.5773	0.03588	135.533908	C_7	133.75	133.6
	130.135	129.7953	0.1764	129.954326	130.3126	0.04557	130.260807	C_8	127.7	129.8
	43.607	43.13	0.1497	43.3310068	43.5687	0.05107	43.5937234	C_5	43.62	43.3
	40.822	40.3534	0.1381	40.5488278	40.7788	0.11418	40.819896	C_6 (CH)	43.08	40.3
	40.758	40.1838	0.1349	40.4154598	40.7633	0.07475	40.7784506	C_3	40.13	40
	39.152	38.6569	0.1335	38.8605563	39.114	0.09464	39.1488306	C_{13}	34.95	33.3
	35.114	34.7064	0.1232	34.877088	35.0713	0.06837	35.1017992	C_9	34.33	36.2
	23.194	22.8644	0.1251	23.0082203	23.2218	0.08668	23.2317897	C_{10}	22.71	23.3
	30.123	29.7546	0.1457	29.9166868	30.2164	0.07697	30.2012207	C_4 (CH)	30.67	30.8
	20.718	20.3621	0.1293	20.5160808	20.8498	0.0779	20.8213923	C_{14}	20	20.6
	20.409	20.0608	0.1274	20.2116535	20.5006	0.07979	20.4866922	C_2	20.17	20.2
	14.489	14.3661	0.0329	14.4165998	14.6098	0.05452	14.5799233	C_{15}	14.1	14.5
	14.327	14.1981	0.0511	14.2548403	14.4611	0.05573	14.4268436	C_1	14.52	14.4
	13.7154	13.5924	0.0406	13.6446865	13.7922	0.0574	13.7783785	C_{11}	13.72	14.2
	19.3375	19.1897	0.0434	19.2513035	19.4234	0.02471	19.3989565	C_{12}	20.44	21.4
C5-A'	135.7706	135.5615	0.1549	135.669925	135.9451	0.04063	135.893268	C_7	133.75	133.6
	129.8569	129.5182	0.176	129.676785	130.0145	0.03747	129.967864	C_8	127.7	129.8
	43.985	43.4769	0.135	43.6854475	43.9366	0.06192	43.9676268	C_5	43.62	43.3
	40.6382	40.0505	0.1306	40.2859065	40.6339	0.07076	40.6515029	C_6 (CH)	43.08	40.3
	38.8754	38.5599	0.17	38.709	38.8946	0.11239	38.9134487	C_3	40.13	40
	38.384	37.8624	0.031	38.0520125	38.3208	0.07965	38.3610404	C_{13}	34.95	33.3
	35.1426	34.7322	0.1244	34.904141	35.111	0.07544	35.1392226	C_9	34.33	36.2
	23.2126	22.8759	0.124	23.021955	23.2468	0.08332	23.2537853	C_{10}	22.71	23.3
	30.0587	29.6737	0.1463	29.8417333	30.121	0.07598	30.1164805	C_4 (CH)	30.67	30.8
	20.6487	20.2937	0.1291	20.4473203	20.7827	0.07666	20.7532402	C_{14}	20	20.6
	20.2268	19.8696	0.1175	20.0213513	20.3157	0.08346	20.3035722	C_2	20.17	20.2
	14.5624	14.4349	0.0363	14.4877833	14.6855	0.05484	14.6548911	C_{15}	14.1	14.5
	14.3463	14.2221	0.0301	14.2724178	14.4789	0.05586	14.4451982	C_1	14.52	14.4
	13.7474	13.623	0.0375	13.6750713	13.8276	0.05655	13.8123951	C_{11}	13.72	14.2
	20.5958	20.3667	0.0277	20.4531868	20.6554	0.02588	20.6404277	C_{12}	20.44	21.4
C5-B	135.6656	135.6223	0.199	135.682728	135.8707	0.05813	135.81214	C_7	138.4	133.6
	129.1638	128.9014	0.156	129.02873	129.3322	0.04363	129.283186	C_8	124.6	129.8
	44.4929	43.9602	0.124	44.174855	44.4277	0.07586	44.4677782	C_5	43.62	30.8
	39.2667	38.9202	0.162	39.07833	39.2707	0.11451	39.295351	C_3	40.13	40
	38.7484	38.1807	0.112	38.404875	38.6705	0.09053	38.7183606	C_{13}	34.95	33.3
	34.8995	34.4971	0.147	34.6713825	34.976	0.09326	34.9704417	C_6 (CH)	43.08	34.3
	23.4233	23.0949	0.123	23.2378225	23.4804	0.06791	23.4758645	C_{10}	22.98	23.3
	30.4178	30.0406	0.151	30.2069725	30.4728	0.07954	30.4716454	C_4 (CH)	30.67	30.8
	20.7597	20.4241	0.134	20.572045	20.8824	0.06734	20.8547749	C_{14}	20	20.6
	20.4362	20.0579	0.109	20.2151025	20.5096	0.08602	20.5034796	C_2	20.17	20.2
	30.2735	29.8973	0.137	30.0601375	30.3157	0.04593	30.3113791	C_9	29.43	30.2
	14.5979	14.4647	0.039	14.5201925	14.7214	0.04918	14.6893635	C_{15}	14.1	14.5
	14.4854	14.3412	0.021	14.3964475	14.5963	0.06833	14.5730301	C_1	14.52	14.4
	14.037	13.9736	0.051	14.0073925	14.1216	0.01911	14.0963375	C_{11}	13.85	14.2
	20.628	20.3934	0.038	20.484155	20.6775	0.02312	20.6654348	C_{12}	20.44	21.4
C5-B'	135.3633	135.2921	0.193	135.360928	135.5419	0.05747	135.492464	C_7	138.4	133.6
	129.5604	129.2847	0.152	129.415775	129.7553	0.04618	129.697591	C_8	124.6	129.8
	44.0589	43.563	0.143	43.7690975	43.9976	0.06063	44.0328483	C_5	43.62	30.8
	40.822	40.3573	0.137	40.5511125	40.779	0.11418	40.820026	C_3	40.13	40
	39.437	38.929	0.145	39.1397875	39.39	0.108	39.43102	C_{13}	34.95	33.3
	35.0053	34.5844	0.19	34.77494	35.069	0.09158	35.0675395	C_6 (CH)	43.08	34.3
	23.4613	23.1409	0.137	23.2842075	23.5277	0.0714	23.5207035	C_{10}	22.98	23.3
	30.3143	29.9957	0.18	30.14816	30.4061	0.0835	30.3929663	C_4 (CH)	30.67	30.8
	20.7744	20.428	0.146	20.582455	20.8895	0.06665	20.8643779	C_{14}	20	20.6
	20.4045	20.058	0.136	20.210215	20.4832	0.09551	20.4773835	C_2	20.17	20.2
	30.3143	29.9518	0.15	30.1128	30.3662	0.0484	30.359046	C_9	29.43	30.2
	14.4917	14.3749	0.042	14.425335	14.6161	0.03574	14.5806909	C_{15}	14.1	14.5
	14.4662	14.3221	0.03	14.37936	14.5846	0.05807	14.5563709	C_1	14.52	14.4
	14.0212	13.9405	0.051	13.9803475	14.1135	0.02077	14.0859202	C_{11}	13.85	14.2
	19.7285	19.5375	0.047	19.6150425	19.8074	0.03229	19.787131	C_{12}	20.44	21.4
C5-C	147.91925	148.8897	0.4575	148.654124	148.6535	0.17459	148.436232	C_4	148.1	152.6
	110.85538	110.1453	-0.02	110.389278	110.90033	-0.08316	110.865679	C_{12}	111.3	107.9
	41.58304	41.275	0.185	41.4249015	41.62296	0.06716	41.6242669	C_5	41.83	42.8
	38.18632	37.8351	0.283	38.0224095	38.21157	0.09688	38.2247727	C_3	39.29	39.8
	35.43145	35.0412	0.211	35.22579	35.48884	0.0901	35.4892513	C_6 (CH)	37.25	35.3
	33.78525	33.4052	0.204	33.5846275	33.84872	0.0939	33.8478678	C_7	33.1	33.4
	36.24872	35.8502	0.197	36.0344995	36.2769	0.08601	36.2866043	C_{13}	32.21	36.2
	23.05798	22.7146	0.1665	22.8726618	23.11634	0.10706	23.1202702	C_{10}	22.75	22.7
	32.7448	32.3334	0.186	32.519705	32.74873	0.12772	32.7764108	C_9	32.2	32.1
	21.12594	20.8385	0.176	20.979144	21.19791	0.08861	21.1928793	C_2	20.82	20.8
	20.02217	19.6998	0.176	19.8526695	20.11595	0.06774	20.0985379	C_{14}	20.38	20.6
	26.57891	26.1981	0.203	26.377566	26.64195	0.0995	26.6425223	C_8	27.3	27.2
	14.61368	14.498	0.045	14.5487255	14.74382	0.04436	14.7083629	C_{15}	14.17	14.4
	14.25201	14.1262	0.045	14.180471	14.35831	0.05714	14.3341044	C_{11}	14.15	14.1

C6-C5 neat	CDCl3	C6D6	increment	C8 trimer isomer	C8 trimer* neat	C8-C6 neat-C6	increment	
-0.192	-0.1594	-0.1483	εε$^{\pi}$	C8-A	135.201	-0.037		0
0.113	0.1657	0.2054	δ		130.263	0.015	ε	
0.019	0.048	0.0913	εε		43.569	-0.057		0
0.106	0.0566	0.2522	δ		40.923	-0.005	ε	
-2.614	-2.4508	-2.5343	γ		38.427	0.283	δε	
-2.634	-2.5679	-2.489	γ		36.796	0.278	δε	
-2.507	-2.4484	-2.3793	γ		32.876	0.269	δε	
9.096	9.0756	9.0722	β		30.311	-1.979	γδ	
0.208	0.2594	0.3046	δ		30.328	-0.003	ε	
9.192	9.1819	9.1972	β		27.605	-2.305	γδ	
9.233	9.2182	9.2284	β		27.337	-2.305	γδ	
8.829	8.6469	8.8412	α		30.027	6.709	βγ	
8.806	8.6339	8.8289	α		29.818	6.685	βγ	
8.6956	8.5166	8.7028	α		29.07	6.659	βγ	
0.0455	0.0633	0.0896	ε		19.37	-0.013		0
					32.333	18.05	αβ	
					32.308	18.053	αβ	
					32.123	18.079	αβ	
-0.2126	-0.1755	-0.1541	εε$^{\pi}$	C8-A'	135.524	-0.034		0
0.1501	0.1918	0.2265	δ		130.009	0.002	ε	
-0.02	0.0101	0.0504	εε		43.911	-0.054		0
0.1428	0.2065	0.2511	δ		40.769	-0.012	ε	
-2.7724	-2.7029	-2.6296	γ		36.357	0.254	δε	
-2.631	-2.6084	-2.4958	γ		36.043	0.29	δε	
-2.4926	-2.4382	-2.374	γ		32.918	0.268	δε	
9.1124	9.0641	9.0772	β		30.044	-2.281	γδ	
0.2083	0.2533	0.302	δ		30.221	-0.046	ε	
9.1743	9.1633	9.1823	β		27.683	-2.14	γδ	
9.2092	9.1864	9.2003	β		27.507	-1.929	γδ	
8.8146	8.6041	8.7965	α		29.95	6.573	βγ	
8.7957	8.6279	8.8221	α		29.827	6.685	βγ	
8.7066	8.526	8.7084	α		29.12	6.666	βγ	
0.0372	0.0553	0.0816	ε		20.635	0.002		0
					32.352	18.059	αβ	
					32.308	18.054	αβ	
					32.137	18.073	αβ	
-0.1816	-0.1193	-0.1127	εε$^{\pi}$	C8-B	135.393	-0.091		0
0.1552	0.1956	0.2278	δ		129.338	0.019	ε	
-0.0079	0.0228	0.0563	εε		44.445	-0.04		0
-2.7037	-2.6442	-2.5817	γ		36.796	0.233	δε	
-2.6564	-2.5947	-2.5275	γ		36.4	0.308	δε	
0.1125	0.1759	0.201	δ		35.01	-0.002	ε	
9.1377	9.0951	9.0996	β		30.105	-2.456	γδ	
0.2092	0.2604	0.3012	δ		30.593	-0.034	ε	
9.1563	9.1409	9.1516	β		27.643	-2.273	γδ	
9.2318	9.2121	9.2174	β		27.337	-2.331	γδ	
-2.4035	-2.3763	-2.2977	γ		28.14	0.27	δε	
8.8701	8.6833	8.8806	α		30.053	6.585	βγ	
8.7746	8.6168	8.8097	α		29.887	6.627	βγ	
8.77	8.5394	8.7614	α		29.548	6.741	βγ	
0.067	0.0796	0.1095	ε		20.701	0.006		0
					32.333	18.028	αβ	
					32.308	18.052	αβ	
					32.217	18.072	αβ	
-0.1733	-0.1111	-0.0979	εε$^{\pi}$	C8-B'	135.137	-0.053		0
0.1136	0.1623	0.1917	δ		129.689	0.015	ε	
-0.0009	0.033	0.0704	εε		44.038	-0.02		0
-2.676	-2.6243	-2.554	γ		38.412	0.266	δε	
-2.688	-2.614	-2.554	γ		37.027	0.278	δε	
0.1397	0.2016	0.227	δ		35.144	-0.001	ε	
9.1377	9.0951	9.1013	β				γδ	
0.2257	0.2763	0.3139	δ		30.514	-0.026	ε	
9.1716	9.155	9.1625	β				γδ	
9.2085	9.2	9.2118	β		27.293	-2.32	γδ	
-2.4373	-2.3988	-2.3272	γ		28.179	0.302	δε	
8.8493	8.6581	8.5439	α		30.027	6.686	βγ	
8.7838	8.6189	8.8124	α		30.013	6.763	βγ	
8.7428	8.5435	8.7295	α		29.472	6.708	βγ	
0.0345	0.0635	0.0936	ε		19.77	0.007		0
					32.333	18.052	αβ	
					32.308	18.053	αβ	
					32.196	18.036	αβ	
0.22275	0.2723	0.2935	δ	C8-C	148.1	-0.042	ε	
-0.17438	-0.1643	-0.13733	ε$^{\pi}$		110.642	-0.039		0
0.00196	0.036	0.09704	εε		41.55	-0.035		0
-2.50432	-2.4241	-2.36657	γ		35.947	0.265	δε	
0.11955	0.1828	0.22416	δ		35.507	-0.044	ε	
0.01275	0.0528	0.09028	εε		33.768	-0.03		0
-2.76972	-2.7072	-2.6379	γ		33.752	0.273	δε	
9.26702	9.2314	9.24066	β		30.182	-2.143	γδ	
-2.4378	-2.3474	-2.37673	γ		30.478	0.171	δε	
9.01206	8.9205	9.03809	β		30.053	-0.085	γδ	
9.11783	9.1112	9.13005	β		26.813	-2.327	γδ	
0.27609	0.3239	0.35805	δ		26.838	-0.017	ε	
8.80532	8.625	8.81718	α		30.027	6.608	βγ	
8.79099	8.5818	8.76469	α		29.753	6.71	βγ	

* two sets of three signals for terminal Et groups not resolved at:
14.20-14.26
22.95-23.05

	22.788	22.526	0.181	22.6588775		22.874	0.084	22.86301	C_3	22.53	23.1		13.994	13.9182	0.054	13.957015	14.06599	0.04023	14.0499458	C_1	13.87	14.5	8.794	8.6078	8.80801	α		29.463	6.675	βγ			
	14.274	14.171	0.062	14.221155				4.9959	C_{16}	14.3	14.1																	32.333	18.059	αβ			
	14.239	14.12	0.056	14.17439				4.98365	C_{13}	14.05	14.1																	32.308	18.069	αβ			
	14.14	14.02	0.072	14.07838		14.23	0.03	14.205325	C_1	13.98	14.2																	32.261	18.121	αβ			
C6-D	152.171	153.132	0.299	152.863673	2-^{13}C	152.891	-0.052	152.62717	C_3	152.57	151.2	C5-D	151.9982	152.8878	0.254	152.634225	152.6216	0.1604	152.439901	C_4	152.57	148.6	0.1728	0.2442	0.2694	δε	C8-D	152.125	-0.046	ε			
	109.168	108.382	0.05	108.668475	1-^{13}C	109.217	-0.091	109.179148	C_{13}	107.3	111.8		109.2617	108.4781	0.002	108.752815	109.2521	-0.05248	109.243521	C_{11}	107.3	111.9	-0.0937	-0.0961	-0.0351	ε*		109.139	-0.029		0		
	44.485	44.098	0.233	44.2864575	2-^{13}C	44.651	0.045	44.6031375	C_5 (CH)	46.46	42.3		44.33582	43.8703	0.21	44.081007	44.40319	0.1029	44.4030203	C_5 (CH)	46.46	42	0.14918	0.2277	0.24781	δε		44.445	-0.04	ε			
	42.633	42.253	0.218	42.435595	1-^{13}C	42.695	0.03	42.680125	C_7	33.4	31.5		42.60434	42.1974	0.203	42.3860115	42.5818	0.05568	42.6023562	C_6	33.4	40.8	0.02866	0.0556	0.1132	εε		42.563	-0.07		0		
	36.547	36.279	0.207	36.4198925		36.671	0.082	36.646255	C_9	36.43	40.8		39.28155	38.9518	0.206	39.1140775	39.2865	0.12966	39.3142652	C_8	39.15	40	-2.73455	-2.6728	-2.6155	γ		36.796	0.249	δε			
	34.063	33.613	0.206	33.817365		34.152	0.026	34.126765	C_{14}	33.4	33		36.70993	36.2004	0.186	36.4210505	36.66147	0.06182	36.6924951	C_{12}	31.8	35.5	-2.64693	-2.5874	-2.50947	γ		34.365	0.302	δε			
	32.419	32.253	0.184	32.35296		32.607	-0.016	32.53756	C_2	33.64	37.5		34.945	34.7305	0.218	34.85517	34.99965	0.0736	34.9972665	C_3	35.15	37.3	-2.526	-2.4775	-2.39265	γ		32.691	0.272	δε			
	30.514	30.212	0.207	30.3647925	2-^{13}C	30.675	0.016	30.62229	C_2 (CH)	30.36	30		30.29328	29.9483	0.205	30.1156805	30.36492	0.08628	30.3594747	C_2 (CH)	30.36	31.1	0.22072	0.2637	0.31008	δ		30.426	-0.088	ε			
	30.444	30.1	0.196	30.26499		30.504	0.051	30.4946025	C_3	30.43	31.4		21.27617	20.9482	0.166	21.1007545	21.34017	0.0835	21.3367663	C_2	20.49	21.1	9.16783	9.1518	9.16383	β		28.01	-2.434	γδ			
	30.013	29.716	0.225	29.8711375		30.165	0.043	30.1215825	C_{15}	30	29.9		20.87299	20.5784	0.184	20.7233665	21.00692	0.0733	20.9767203	C_{13}	20.57	20.9	9.14001	9.1376	9.15808	β		27.694	-2.319	γδ			
	29.523	29.142	0.203	29.3215325		29.598	0.094	29.593135	C_{10}	29.2	29.3		20.31163	19.9561	0.162	20.1173905	20.39694	0.0927	20.3881708	C_9	19.61	20.2	9.21137	9.1859	9.20106	β		27.176	-2.347	γδ			
	23.341	23.064	0.227	23.2125925		23.493	0.08	23.458	$C_{16(11)}$	23	23.1		14.55908	14.4398	0.054	14.493833	14.68559	0.05834	14.6545839	C_{14}	14.22	14.5	8.78192	8.6242	8.80741	α		30.013	6.672	βγ			
	23.199	22.911	0.181	23.0529775		23.346	0.078	23.312295	$C_{2(16)}$	22.97	23		14.41757	14.2906	0.045	14.345277	14.53345	0.05557	14.5055342	C_1	13.38	14.5	8.78143	8.6204	8.81255	α		29.957	6.758	βγ			
	23.053	22.776	0.184	22.91481		23.125	0.082	23.118455	$C_{1(2)}$	22.87	22.8		14.30551	14.1968	0.051	14.246451	14.35618	0.03621	14.3466833	C_{10}	14.19	14.4	8.74749	8.5792	8.76882	α		29.722	6.669	βγ			
	20.517	20.311	0.058	20.396295	1-^{13}C	20.606	-0.02	20.5703	C_{18}	19.61	21.4		20.47239	20.2491	0.057	20.340219	20.51215	0.01827	20.5023904	C_{15}	19.96	21.4	0.04461	0.0619	0.09385	ε		20.522	0.005		0		
	14.287	14.175	0.057	14.2271675				5.00045	C_{12}	14.4	14.2																	32.333	18.046	αβ			
	14.223	14.117	0.059	14.1675225		14.371	0.005	14.3203375	C_{17}	14.3	14.1																	32.308	18.085	αβ			
	14.214	14.102	0.053	14.1532575		14.299	0.014	14.272435	C_1	14.17	14.1																	32.294	18.08	αβ			
C6-D'	151.525	152.448	0.277	152.187968	2-^{13}C	152.228	-0.058	151.968755	C_3	152.57	151.1	C5-D'	151.3568	152.1748	0.422	151.984505	151.961	0.1305	151.779219	C_4	152.57	148.6	0.1682	0.2732	0.267	δε	C8-D'	151.453	-0.072	ε			
	109.571	108.81	0.068	109.09182	1-^{13}C	109.622	-0.066	109.589135	C_{13}	107.3	111.8		109.6406	108.8859	0.0125	109.152889	109.6213	-0.00994	109.625794	C_{11}	107.3	111.9	-0.0696	-0.0759	0.0007	ε*		109.579	0.008		0		
	44.937	44.549	0.243	44.7400825	2-^{13}C	45.078	0.058	45.041845	C_5 (CH)	46.46	42.3		44.708	44.2572	0.218	44.464575	44.762	0.1043	44.7668283	C_5 (CH)	46.46	42	0.229	0.2918	0.316	δε		44.948	0.011	ε			
	41.875	41.48	0.22	41.6683	1-^{13}C	41.9	0.003	41.8919325	C_7	33.4	31.5		41.8687	41.4509	0.205	41.6437675	41.8125	0.0287	41.8386993	C_6	33.4	40.8	0.0063	0.0291	0.0875	εε		41.8	-0.075		0		
	38.111	37.686	0.218	37.884345		38.179	0.106	38.179315	C_9	36.43	40.8		40.8333	40.3553	0.181	40.5637775	40.7791	0.0973	40.8202058	C_8	39.15	40	-2.7223	-2.6693	-2.6001	γ		38.378	0.267	δε			
	34.91	34.517	0.209	34.7020975		35.018	0.051	34.9918025	C_{14}	33.4	33		37.58012	37.109	0.192	37.317572	37.53994	0.097	37.5760705	C_{12}	31.8	35.5	-2.67012	-2.592	-2.52194	γ		35.165	0.255	δε			
	31.565	31.366	0.184	31.47751		31.749	0.035	31.6925625	C_2	33.64	37.5		34.1729	33.9108	0.187	34.0450775	34.2212	0.09122	34.2250476	C_3	35.15	37.3	-2.6079	-2.5448	-2.4722	γ				δε			
	30.493	30.17	0.195	30.3274125	2-^{13}C	30.515	0.149	30.5411975	C_3 (CH)	30.36	30		30.16731	29.871	0.208	30.0220285	30.2774	0.05258	30.2508305	C_3 (CH)	30.36	31.1	0.32569	0.299	0.2376	δ		30.478	-0.015	ε			
	30.342	30.065	0.266	30.222465		30.415	-0.083	30.3705675	C_3	30.43	31.4		21.19697	20.8669	0.172	21.0215545	21.25873	0.08205	21.2557804	C_2	20.49	21.1	9.14503	9.1981	9.15627	β		27.979	-2.363	γδ			
	30.154	29.844	0.175	29.9923125		30.282	-0.039	30.2283275	C_{15}	30	29.9		20.97358	20.6738	0.183	20.8203555	21.10232	0.06637	21.0723602	C_{13}	20.57	20.9	9.18042	9.1702	9.17968	β		27.862	-2.292	γδ			
	29.615	29.2404	0.199	29.4167825		29.673	0.065	29.6674875	C_{10}	29.2	29.3		20.40603	20.0737	0.141	20.222093	20.48947	0.07629	20.477622	C_9	19.61	20.2	9.20897	9.1667	9.18353	β		27.305	-2.31	γδ			
	23.377	23.089	0.239	23.2441725		23.45	0.08	23.44265	C_{16}	23	23.1		14.52057	14.4243	0.097	14.480062	14.64028	0.0481	14.6093243	C_{14}	14.22	14.5	8.85643	8.6647	8.80972	α				βγ			
	23.167	22.871	0.181	23.0157775		23.316	0.081	23.2822775	$C_{2(11)}$	22.97	23		14.37682	14.2449	0.045	14.3013095	14.50756	0.02762	14.4680846	C_1	13.38	14.5	8.79018	8.6261	8.80844	α				βγ			
	23.087	22.807	0.184	22.94686		23.159	0.073	23.1504075	$C_{1(2)}$	22.87	22.8		14.34108	14.194	0.05	14.256853	14.39722	0.01914	14.3819254	C_{10}	14.19	14.4	8.74592	8.613	8.76178	α				βγ			
	19.672	19.516	0.05	19.581975	1-^{13}C	19.802	-0.024	19.75104	C_{18}	19.61	21.4		19.62718	19.4549	0.057	19.5281655	19.7163	0.03566	19.6932207	C_{15}	19.96	21.4	0.04482	0.0611	0.0857	ε		19.684	0.012		0		
	14.272	14.172	0.057	14.2199675		14.393	0.01	14.352925	C_{12}	14.4	14.2																	32.333	18.061	αβ			
	14.262	14.159	0.057	14.2080175		14.382	0.01	14.342275	C_{17}	14.3	14.1																	32.32	18.058	αβ			
	14.244	14.143	0.057	14.1913175		14.308	0.01	14.287875	C_1	14.17	14.1																	32.308	18.064	αβ			
C6-E	148.43	149.465	0.293	149.169408	2-^{13}C	149.204	-0.024	148.92764	C_3	148.1	155.2	C5-E	148.17647	149.1391	0.467	148.908422	148.87425	0.15325	148.664891	C_7	148.1	152.6	0.25353	0.3259	0.32975	δ	C8-E	148.39	-0.04	ε			
	110.792	110.066	0.026	110.326015	1-^{13}C	110.854	-0.133	110.802043	C_{18}	111.64	107.8		110.93884	110.2096	-0.026	110.458919	110.973	-0.09108	110.940323	C_{15}	111.3	107.9	-0.14684	-0.1436	-0.119	ε*		110.766	-0.026		0		
	39.91	39.626	0.199	39.7706725	2-^{13}C	40.104	0.031	40.0431525	C_5 (CH)	39.57	41.1		39.74801	39.4018	0.209	39.570521	39.86168	0.10035	39.8447251	C_5 (CH)	39.57	40.8	0.16199	0.2242	0.24232	δε		39.791	-0.119	ε			
	37.187	36.889	0.176	37.03334	1-^{13}C	37.348	0.015	37.2950625	C_7	41.34	40.3		37.21999	36.8896	0.16	37.0416365	37.30211	0.06662	37.2885241	C_6	41.34	40.3	-0.03299	-0.0006	0.04589	εε		37.153	-0.034		0		
	35.583	35.338	0.219	35.4735725		35.764	0.027	35.7067925	C_9	36.16	37.3		38.08704	37.78763	0.211	37.940426	38.12649	0.08824	38.1327571	C_3	36.63	37.5	-2.50404	-2.44963	-2.36249	γ		35.848	0.265	δε			
	33.892	33.53	0.192	33.70038	2-^{13}C	34.023	0.018	33.981245	C_5 (CH)	35.87	41.2		33.63138	33.2272	0.199	33.4139355	33.69843	0.09626	33.6968617	C_4 (CH)	35.87	40.9	0.26062	0.3028	0.32457	δε		33.873	-0.019	ε			
	33.717	33.417	0.213	33.5704575		33.841	0.039	33.8064725	C_5	35.25	35		36.33288	36.0075	0.211	36.1693855	36.33303	0.07153	36.3492506	C_8	39.29	39.8	-2.61588	-2.5905	-2.49203	γ		34.005	0.288	δε			
	30.544	30.198	0.218	30.368695		30.696	0.015	30.6462125	C_{16}	29.65	32.8		21.09398	20.7578	0.17	20.914138	21.19296	0.07772	21.1759983	C_9	20.82	20.8	9.45002	9.4402	9.50304	β		28.074	-2.47	γδ			
	30.497	30.111	0.2	30.2916		30.625	0.092	30.60113	C_3	29.24	30		21.27577	20.9478	0.175	21.102402	21.3546	0.05176	21.3387849	C_2	21.5	20.5	9.22123	9.1632	9.2704	β		28.057	-2.44	γδ			
	30.365	30.037	0.219	30.2016225		30.433	0.075	30.4262625	C_{15}	29.3	29.6		21.15707	20.8669	0.177	21.008727	21.22384	0.08879	21.2206702	C_{13}	20.42	20.9	9.20793	9.1701	9.20916	β		27.944	-2.421	γδ			
	30.299	29.97	0.206	30.132015		30.414	0.041	30.3830775	C_{14}	27.9	29.6		33.18941	33.8292	0.193	33.649181	33.29433	0.07182	33.2739471	C_{12}	29	35.3	-2.89041	-3.8592	-2.88033	γ		30.774	0.475	δε			
	23.361	23.082	0.189	23.2226475		23.511	0.08	23.4767	C_2	22.87	23		14.51441	14.4041	0.068	14.4581785	14.65498	0.03402	14.6135201	C_1	14.3	14.4	8.84659	8.6779	8.85602	α		30.154	6.793	βγ			
	23.325	23.053	0.238	23.202345		23.452	0.08	23.42575	C_{18}	22.7	23		14.53154	14.4121	0.074	14.470739	14.63604	0.0392	14.608383	C_{14}	14.16	14.4	8.79346	8.6409	8.81596	α		30.088	6.763	βγ			
	22.788	22.526	0.181	22.6588775		22.873	0.088	22.86327	C_{11}	22.53	23.1		13.99027	13.9189	0.052	13.9557095	14.05506	0.04286	14.0421342	C_{10}	13.87	14.5	8.79773	8.6071	8.81794	α		29.463	6.675	βγ			
	15.649	15.434	0.038	15.517895	1-^{13}C	15.649	-0.042	15.639445	C_{13}	19.14	18.9		15.64018	15.3941	0.04	15.489328	15.6394	-0.00275	15.6390474	C_{11}	19.14	18.9	0.00882	0.0399	0.0096	ε		15.644	-0.005		0		
	14.298	14.19	0.062	14.241905				5.0043	C_1	14.2	14.1																	32.333	18.035	αβ			
	14.267	14.143	0.1	14.20915				4.99345	C_{17}	14.1	14.1																	32.308	18.041	αβ			
	14.136	14.023	0.065	14.0773375		14.228	0.015	14.1992125	C_{12}	13.98	14.2																	32.27	18.134	αβ			
C6-E'	148.324	149.345	0.447	149.089343	2-^{13}C	149.114	-0.009	148.835453	C_3	148.1	155.2	C5-E'	148.09058	149.0612	0.481	148.830911	148.7989	0.1541	148.586046	C_7	148.1	152.6	0.23342	0.2838	0.3151	δ	C8-E'	148.283	-0.041	ε			
	110.802	110.084	0.032	110.34258	1-^{13}C	110.88	-0.148	110.81903	C_{18}	111.64	107.8		110.97671	110.278	-0.104	110.498889	111.01707	-0.08396	110.983843	C_{15}	111.3	107.9	-0.17471	-0.194	-0.13707	ε*		110.766	-0.036		0		
	39.89	39.574	0.284	39.74921	2-^{13}C	40.124	0.004	40.04301	C_5 (CH)	39.57	41.1		39.68721	39.333	0.287	39.522266	39.81313	0.08748	39.7889597	C_5 (CH)	39.57	40.8	0.20279	0.241	0.31087	δε		39.752	-0.138	ε			
	38.57	38.262	0.134	38.400285	1-^{13}C	38.706	0.003	38.6590825	C_7	41.34	40.3		38.55365	38.2209	0.147	38.370805	38.60474	0.05455	38.5992686	C_6	41.34	40.3	0.01635	0.0411	0.10126	εε		38.58	0.01		0		
	35.414	35.166	0.179	35.2935225		35.597	0.037	35.5413675	C_9	36.16	37.3		37.94173	37.6393	0.192	37.7888305	37.98323	0.09233	37.9897101	C_3	36.63	37.5	-2.52773	-2.4733	-2.38623	γ		35.463	0.049	δε			
	33.811	33.466	0.089	33.6069975	2-^{13}C	34.028	-0.019	33.9477275	C_5 (CH)	35.87	41.2		33.61983	33.3074	0.203	33.462933	33.76493	0.08875	33.7343356	C_4 (CH)	35.87	40.9	0.19117	0.1586	0.26307	δε		33.795	-0.016	ε			
	34.089	33.729	0.168	33.89322		34.167	0.026	34.145615	C_5	35.25	35		36.6883	36.38	0.197	36.5327225	36.6456	0.014	36.66373	C_8	39.29	39.8	-2.5993	-2.651	-2.4786	γ		34.365	0.276	δε			
	30.428	30.091	0.162	30.245805		30.481	0.043	30.4722325	C_{16}	29.65	32.8		21.12	20.89	0.025	20.9761875			7.392	C_9	20.82	20.8	9.308	9.201	30.481	β				γδ			
	30.477	30.171	0.149	30.3119975		30.58	0.13	30.573525	C_3	29.24	30		21.2484	20.9255	0.191	21.0819675	21.42533	-0.20138	21.3175906	C_2	21.5	20.5	9.2286	9.2455	9.15467	β				γδ			
	30.661	30.257	-0.069	30.3827025		30.628	0.221	30.6898275	C_{15}	29.3	29.6		21.35765	21.0271	0.164	21.1801025	21.43446	0.0687	21.4232058	C_{13}	20.42	20.9	9.30335	9.2299	9.19354	β				γδ			
	29.31	29.018	0.201	29.1659275		29.504	0.078	29.453845	C_{14}	27.9	29.6		32.06125	31.7027	0.17	31.8668675	32.11277	0.07583	32.1119893	C_{12}	29	35.3	-2.75125	-2.6847	-2.60877	γ				δε			
	23.404	23.032	0.281	23.2261275		23.531	0.11	23.511575	C_2	22.87	23		ca 14			#VALUE!			#VALUE!	C_1	14.3	14.4	#VALUE!	23.032	23.531	α				βγ			
	23.378	23.083	0.157	23.2219675		23.47	0.09	23.458275	C_{18}	22.7	23		ca 14			#VALUE!			#VALUE!	C_{14}	14.16	14.4	#VALUE!	23.083	23.47	α				βγ			
	22.705	22.426	0.167	22.5616425		22.858	0.114	22.830385	C_{11}	22.53	23.1		13.95261	13.8781	0.054	13.9164635	14.04253	0.03928	14.0199942	C_{10}	13.87	14.5	8.75239	8.5479	8.81547	α				βγ			
	15.324	15.166	0.04	15.2304	1-^{13}C	15.465	-0.046	15.405185	C_{13}	19.14	18.9		15.23609	15.0907	0.044	15.1515965	15.33076	-0.00131	15.2973275	C_{11}	19.14	18.9	0.08791	0.0753	0.13424	ε		15.303	-0.021		0		
	ca 14			#VALUE!				#VALUE!	C_1	14.2	14.1																			αβ			
	ca 14			#VALUE!				#VALUE!	C_{17}	14.1	14.1																			αβ			
	ca 14			#VALUE!				#VALUE!	C_{12}	13.98	14.2																			αβ			
C6-F	130.174	130.215	0.206	130.247515	2-^{13}C	130.57	-0.109	130.406603	C_3	131.36	130.6	C5-F	130.024	130.011	0.213	130.064008	130.29107	0.07944	130.215668	C_8	132	128	0.15	0.204	0.27893	δ	C8-F	130.173	-0.001	ε			
	129.59	129.645	0.248	129.68217	1-^{13}C	129.951	0.017	129.828518	C_8	129.31	128.6		129.827	129.851	0.211	129.890603	130.14334	0.13551	130.06345	C_7	129.31	128.7	-0.237	-0.206	-0.19234	ε*		129.52	-0.07		0		
	43.359	43.025	0.212	43.19013	2-^{13}C	43.524	0.01	43.468525	C_5 (CH)	39.57	43.6		43.16	42.791	0.189	42.9631475	43.23078	0.08872	43.2261908	C_5 (CH)	39.57	43.3	0.199	0.234	0.29322	δε		43.316	-0.043	ε			
	34.042	33.721	0.179	33.8740725		34.133	0.019	34.1054725	C_5	36.13	35		36.677	36.309	0.166	36.475565	36.76264	0.07223	36.7490983	C_3	36.63	37.5	-2.635	-2.588	-2.62964	γ		34.304	0.262	δε			
	34.567	34.185	0.228	34.37057	2-^{13}C	34.692	0.007	34.6498425	C_5 (CH)	35.87	40.9		34.347	33.93	0.162	34.112805	34.3869	0.077	34.3904525	C_4 (CH)	35.87	40.6	0.22	0.255	0.3051	δ		34.546	-0.021	ε			
	32.355	31.995	0.116	32.14739		32.348	0.01	32.352725	C_{16}	27.9	32.5		35.117	34.721	0.136	34.89054	35.05	0.1	35.0962	C_{13}	27.9	35	-2.762	-2.726	-2.702	γ				δε			
	32.291	31.956	0.18	32.1142		32.301	0.01	32.299775	C_{11}	31.65	32.1		23.227	22.911	0.124	23.04981	23.28	0.1	23.2842	C_{10}	22.7	23.3	9.064	9.045	9.021	β				γδ			
	28.007	27.681	0.175	27.8349125	1-^{13}C	28.315	-0.034	28.199465	C_7	32.27	33.5		28.064	27.735	0.123	27.8781325	28.20537	0.0412	28.1652635	C_6	32.27	33.5	-0.057	-0.054	0.10963	ε		28.109	0.102		0		
	30.995	30.676	0.179	30.8283725		31.167	0.004	31.10771	C_3	29.24	29.6		22.661	22.39	0.352	22.56493	22.784	0.1	22.7637	C_2	21.5	20.5	8.334	8.286	8.383	β				γδ			
	29.917	29.559	0.163	29.7213825		29.68	0.82	29.9495	C_{18}	29.3	30		21.282	20.96	0.049	21.0838475			7.4487	C_{14}	20.42	20.9	8.635	8.599	29.68	β		27.466	-2.451	γδ			
	27.379	27.09	0.151	27.2255025		27.557	0.021	27.4994775	C_{16}	26.43	27.4		29.775	29.462	0.147	29.6049925	29.829	0.1	29.83285	C_9	29.5	29.9	-2.396	-2.372	-2.272	γ				δε			

	ca 23			#VALUE!			#VALUE!	C_{17}	22.7	23		ca 14			#VALUE!			#VALUE!	C_{15}	14.16	14.4		#VALUE!	0	0	α					βγ							
	ca 23			#VALUE!			#VALUE!	C_2	22.87	23		ca 14			#VALUE!			#VALUE!	C_1	14.3	14.4		#VALUE!	0	0	α					βγ							
	ca 23			#VALUE!			#VALUE!	C_{12}	22.12	22.8		ca 14			#VALUE!			#VALUE!	C_{11}	13.8	14.2		#VALUE!	0	0	α					βγ							
	15.869	15.648	0.043	15.7351325	$1-^{13}C$	15.93	-0.033	15.9011425	C_{14}	19.14	16.6		15.848	15.629	0.031	15.7127025	15.86405	0.00139	15.8587487	C_{12}	19.14	18.9		0.021	0.019	0.06595	εε		15.879	0.01		0							
	ca 14			#VALUE!			#VALUE!	C_1	14.2	14.1																				αβ							
	ca 14			#VALUE!			#VALUE!	C_{13}	13.72	14.2																				αβ							
	ca 14			#VALUE!			#VALUE!	C_{16}	14.1	14.1																				αβ							
C6-F'	130.285	130.305	0.212	130.34623	$2-^{13}C$	130.681	-0.113	130.516693	C_9	131.36	130.6	C5-F'	130.14	130.113	0.191	130.165903	130.41	0.08	130.3337	C_8	132	128		0.145	0.192	0.271	δ	C8-F'			ε							
	129.416	129.505	0.184	129.51571	$1-^{13}C$	129.787	0.019	129.661473	C_8	129.31	128.6		129.667	129.699	0.219	129.737623	129.8005	0.14	129.785625	C_7	129.31	128.7		-0.251	-0.194	-0.0135	ε*		129.353	-0.063		0							
	43.323	43.014	0.255	43.1801625	$2-^{13}C$	43.5	-0.004	43.43714	C_6 (CH)	39.57	43.6		43.134	42.787	0.186	42.950765	43.20042	0.07636	43.1945449	C_6 (CH)	39.57	43.3		0.189	0.227	0.29958	δε		43.272	-0.051	ε							
	34.155	33.765	0.164	33.93881		34.252	0.046	34.228515	C_9	36.13	35		36.604	36.218	0.158	36.389045	36.66	0.1	36.66315	C_3	36.63	37.5		-2.449	-2.453	-2.408	γ		34.422	0.267	δε							
	34.5	34.156	0.244	34.33191	$2-^{13}C$	34.661	0.001	34.6048775	C_3 (CH)	35.87	40.9		34.257	33.904	0.181	34.0687275	34.33791	0.10069	34.3324985	C_4 (CH)	35.87	40.6		0.243	0.252	0.32309	δ		34.513	0.013	ε							
	32.241	31.87	0.164	32.03716				11.28435	C_{10}	27.9	32.5		34.583	34.129	0.149	34.3217975	34.462	0.066	34.519365	C_{13}	27.9	35		-2.342	-2.259	-34.462	γ				δε							
	32.213	31.85	0.193	32.0209575		32.24	0.1	32.2533	C_{11}	31.65	32.1		23.235	23.92	0.127	23.7091425	23.295	0.1	23.29675	C_{10}	22.7	23.3		8.978	7.93	8.945	β				γδ							
	29.316	28.99	0.13	29.133675	$1-^{13}C$	29.455	0.121	29.4338775	C_7	32.27	33.5		29.369	29.015	0.124	29.16711	29.48082	0.07929	29.4597215	C_6	32.27	33.5		-0.053	-0.025	-0.02582	ε					0						
	30.758	30.445	0.17	30.593225				10.7653	C_3	29.24	29.6		21.461	21.126	0.132	21.27328			7.51135	C_2	21.5	20.5		9.297	9.319	0	β				γδ							
	30.492	30.151	0.283	30.3347325				10.6722	C_{16}	29.3	30		21.186	20.838	0.163	20.9968825			7.4151	C_{14}	20.42	20.9		9.306	9.313	0	β				γδ							
	27.379	27.096	0.154	27.230085		27.567	0.0077	17.9203018	C_{15}	26.43	27.4		29.958	29.606	0.148	29.76287	29.874	0.1	29.92615	C_9	29.5	29.9		-2.579	-2.51	-2.307	γ				δε							
	ca 23			#VALUE!			#VALUE!	C_{17}	22.7	23		ca 14			#VALUE!			#VALUE!	C_{15}	14.16	14.4		#VALUE!	0	0	α					βγ							
	ca 23			#VALUE!			#VALUE!	C_2	22.87	23		ca 14			#VALUE!			#VALUE!	C_1	14.3	14.4		#VALUE!	0	0	α					βγ							
	ca 23			#VALUE!			#VALUE!	C_{12}	22.12	22.8		ca 14			#VALUE!			#VALUE!	C_{11}	13.8	14.2		#VALUE!	0	0	α					βγ							
	15.728	15.56	0.047	15.6294925	$1-^{13}C$	15.809	-0.052	15.76882	C_{14}	19.14	16.6		15.65	15.48	0.049	15.5506475	15.68366	-0.03048	15.6649448	C_{12}	19.14	18.9		0.078	0.08	0.12534	εε		15.732	0.004		0							
	ca 14			#VALUE!			#VALUE!	C_1	14.2	14.1																				αβ							
	ca 14			#VALUE!			#VALUE!	C_{13}	13.72	14.2																				αβ							
	ca 14			#VALUE!			#VALUE!	C_{16}	14.1	14.1																				αβ							
C6-G	131.239	131.19	0.174	131.246735	$2-^{13}C$	131.592	-0.116	131.44206	C_9	131.8	130.6	C5-G	131.101	130.991	0.197	131.074318	131.306	0.14496	131.267228	C_8	131.8	128		0.138	0.199	0.286	δ	C8-G	131.227	-0.012	ε							
	130.121	130.03	0.12	130.08915	$1-^{13}C$	130.402	0.014	130.306835	C_8	128.7	128.6		130.341	130.205	0.182	130.294005	130.7523	-0.28975	130.542427	C_7	128.7	128.7		-0.22	-0.175	-0.3503	ε*		130.071	-0.05		0						
	42.93	42.923	0.068	42.94092	$2-^{13}C$	43.072	-0.015	43.0188875	C_6 (CH)	39.57	43.6		42.738	42.373	0.18	42.5417	42.755	0.49132	42.8608253	C_6 (CH)	39.57	43.3		0.192	0.55	0.317	δε		42.88	-0.05	ε							
	33.96	33.563	0.28	33.76565		34.074	0.043	34.0438825	C_9	36.13	35		36.524	36.019	0.146	36.228965	36.573	0.244	36.61136	C_3	36.63	37.5		-2.564	-2.456	-2.499	γ		34.204	0.244	δε							
	34.516	34.12	0.172	34.29773	$2-^{13}C$	34.615	0.013	34.5833075	C_3 (CH)	35.87	40.9		34.258	33.822	0.151	34.0089525	34.251	0.10796	34.2780109	C_4 (CH)	35.87	40.6		0.258	0.298	0.364	δ		34.479	-0.037	ε							
	32.565	32.2	0.16	32.36415		32.584	0.045	32.5875875	C_{16}	27.9	32.5		35.209	34.818	0.119	34.9819225	35.105	0.05	35.152775	C_{13}	27.9	35		-2.644	-2.618	-2.521	γ				δε							
	32.247	31.878	0.178	32.047645		32.248	0.113	32.2733575	C_{11}	32.26	32.1		23.127	22.797	0.151	22.9468525	23.205	-0.025	23.1720125	C_{10}	22.93	23.3		9.12	9.081	9.043	β				γδ							
	33.717	33.361	-0.159	33.4494275	$1-^{13}C$	33.849	-0.029	33.7962025	C_7	32.27	39.5		33.554	33.151	0.148	33.32572	33.859	0.31686	33.8243351	C_6	32.27	39.5		0.163	0.21	-0.01	ε					0						
	30.827	30.471	0.17	30.634275		30.998	0.005	30.9392875	C_3	29.24	29.6		21.414	21.069	0.128	21.21887	21.174	0.1	21.28075	C_2	21.5	20.5		9.413	9.402	9.824	β				γδ							
	30.305	29.981	0.132	30.12443		30.362	0.018	30.346145	C_{16}	29.3	30		ca 21.1			#VALUE!			#VALUE!	C_{14}	20.42	20.9		#VALUE!	29.981	30.362	β				γδ							
	32.723	32.363	0.124	32.51721		32.824	-0.011	32.7861475	C_{15}	32.54	33.4		35.344	34.843	0.382	35.105255	35.383	0.1	35.3921	C_9	34.43	35.9		-2.621	-2.48	-2.559	γ				δε							
	ca 23			#VALUE!			#VALUE!	C_{17}	22.7	23		ca 14			#VALUE!			#VALUE!	C_{15}	14.16	14.4		#VALUE!	0	0	α					βγ							
	ca 23			#VALUE!			#VALUE!	C_2	22.87	23		ca 14			#VALUE!			#VALUE!	C_1	14.3	14.4		#VALUE!	0	0	α					βγ							
	ca 23			#VALUE!			#VALUE!	C_{12}	22.62	22.8		ca 14			#VALUE!			#VALUE!	C_{11}	13.55	14.2		#VALUE!	0	0	α					βγ							
	15.837	15.663	-0.056	15.71116	$1-^{13}C$	15.912	-0.05	15.874375	C_{14}	19.14	18.9		15.825	15.64	0.041	15.7140775	15.854	0.0147	15.8471943	C_{12}	19.14	18.9		0.012	0.023	0.058	εε		15.849	0.012		0							
	ca 14			#VALUE!			#VALUE!	C_1	14.2	14.1																				αβ							
	ca 14			#VALUE!			#VALUE!	C_{13}	13.9	14.2																				αβ							
	ca 14			#VALUE!			#VALUE!	C_{16}	14.1	14.1																				αβ							
C6-G'	131.266	131.201	0.19	131.266975	$2-^{13}C$	131.618	-0.108	131.47023	C_9	131.8	130.6	C5-G'	131.129	131.009	0.191	131.094453	131.366	0.02379	131.288462	C_8	131.8	128		0.137	0.192	0.252	δ	C8-G'	131.259	-0.007	ε							
	129.95	129.866	0.155	129.930663	$1-^{13}C$	130.236	0.04	130.145	C_8	128.7	128.6		130.186	130.059	0.179	130.144173	130.435	0.1	130.3706	C_7	128.7	128.7		-0.236	-0.193	-0.199	ε*		129.897	-0.053		0						
	43.017	42.754	0.109	42.8708475	$2-^{13}C$	43.203	-0.009	43.1358525	C_6 (CH)	39.57	43.6		42.803	42.442	0.201	42.6140775	42.748	0.1	42.79	C_6 (CH)	39.57	43.3		0.214	0.312	0.455	δε		42.941	-0.076	ε							
	34.112	33.741	0.171	33.9097525				11.9392	C_9	36.13	35		36.811	36.394	0.153	36.5747575	36.826	0.01	36.823025	C_3	36.63	37.5		-2.699	-2.653	-36.826	γ		34.468	0.356	δε							
	34.417	34.072	0.198	34.237795	$2-^{13}C$	34.583	-0.008	34.52308	C_3 (CH)	35.87	40.9		34.204	33.795	0.062	33.952255			11.9714	C_4 (CH)	35.87	40.6		0.213	0.277	34.583	δ		34.42	0.003	ε							
	ca 32.15			#VALUE!			#VALUE!	C_{15}	27.9	32.5		33.74	33.405	0.005	33.5233875	33.965	0.1	33.909	C_{13}	27.9	35		#VALUE!	-33.405	-33.965	γ				δε							
	ca 32.2			#VALUE!			#VALUE!	C_{11}	32.26	32.1		23.105	22.78	0.179	22.9344725	23.194	0.1	23.1856	C_{10}	22.93	23.3		#VALUE!	-22.78	-23.194	β				γδ							
	34.977	34.598	0.071	34.7468025	$1-^{13}C$	35.124	-0.017	35.0686825	C_7	32.27	39.5		35.181	34.791	0.146	34.960715	34.897	0.1	35.01915	C_6	32.27	39.5		-0.204	-0.193	0.227	ε					0						
	ca 30.8			#VALUE!			#VALUE!	C_3	29.24	29.6		21.51	21.221	0.108	21.34672			7.5285	C_2	21.5	20.5		#VALUE!	-21.221	0	β				γδ							
	ca 30.3			#VALUE!			#VALUE!	C_{16}	29.3	30		ca 21.1			#VALUE!			#VALUE!	C_{14}	20.42	20.9		#VALUE!	0	0	β				γδ							
	ca 32.6			#VALUE!			#VALUE!	C_{15}	32.54	33.4		35.271	35.023	-0.089	35.0895525			12.34485	C_9	34.43	35.9		#VALUE!	-35.023	0	γ				δε							
	ca 23			#VALUE!			#VALUE!	C_{17}	22.7	23		ca 14			#VALUE!			#VALUE!	C_{15}	14.16	14.4		#VALUE!	0	0	α					βγ							
	ca 23			#VALUE!			#VALUE!	C_2	22.87	23		ca 14			#VALUE!			#VALUE!	C_1	14.3	14.4		#VALUE!	0	0	α					βγ							
	ca 23			#VALUE!			#VALUE!	C_{12}	22.62	22.8		ca 14			#VALUE!			#VALUE!	C_{11}	13.55	14.2		#VALUE!	0	0	α					βγ							
	15.726	15.415	0.25	15.580725	$1-^{13}C$	15.724	-0.04	15.7156	C_{14}	19.14	18.9	15.73	15.534	15.367	0.042	15.435005	15.584	0.0038	15.5673645	C_{12}	19.14	18.9		0.192	0.048	0.14	εε	15.73	15.613	-0.113		0							
	ca 14			#VALUE!			#VALUE!	C_1	14.2	14.1																				αβ							
	ca 14			#VALUE!			#VALUE!	C_{13}	13.9	14.2																				αβ							
	ca 14			#VALUE!			#VALUE!	C_{16}	14.1	14.1																				αβ							
C6-H	151.77	152.772	0.389	152.509798	$2-^{13}C$	152.538	-0.045	152.258963	C_9	152.57	151.2	C5-H	151.612	152.5	0.4466	152.290802	152.4169	0.1	152.157935	C_8	152.57	148.6		0.158	0.272	0.1211	δε	C8-H	151.705	-0.065	ε							
	109.217	108.464	-0.039	108.716678	$1-^{13}C$	109.262	-0.114	109.220315	C_{14}	107.3	111.8		109.306	108.549	-0.027	108.807808	109.4431	0.1	109.417865	C_{12}	107.3	111.9		-0.089	-0.085	-0.1811	ε*		109.212	-0.005		0						
	47.127	46.755	0.285	46.9500375	$2-^{13}C$	47.287	0.047	47.2416925	C_6 (CH)	47.13	44.8		46.969	46.528	0.261	46.7417275	46.834	0.1	46.904	C_6 (CH)	47.13	44.5		0.158	0.227	0.453	δε		47.118	-0.009	ε							
	ca 31.7			#VALUE!			#VALUE!	C_9	33.64	31.5		34.343	33.783	0.121	34.0065275	34.272	0.1	34.3196	C_3	35.15	37.3		#VALUE!	-33.783	-34.272	γ				δε							
	ca 33.0			#VALUE!			#VALUE!	C_{16}	33.4	32.7		35.355	35.149	0.174	35.260685			12.37425	C_{13}	31.8	35.2		#VALUE!	-35.149	0	γ				δε							
	34.567	34.162	0.043	34.3135325	$1-^{13}C$	34.637	0.027	34.6186425	C_7	33.4	33		34.583	34.13	0.148	34.32222	34.444	0.1	34.5154	C_6	33.4	33		-0.016	0.032	0.193	εε					0						
	32			11.2				11.2	C_{11}	31.93	31.9		ca 23			#VALUE!			#VALUE!	C_{10}	22.63	22.7		#VALUE!	0	0	β				γδ							
	30			10.5				10.5	C_3	30.43	29.9		ca 21			#VALUE!			#VALUE!	C_2	20.49	21.1		#VALUE!	0	0	β				γδ							
	30			10.5				10.5	C_{16}	30	30		ca 21			#VALUE!			#VALUE!	C_{14}	20.57	20.9		#VALUE!	0	0	β				γδ							
	ca 30.5	30.25		#VALUE!	$2-^{13}C$			#VALUE!	C_9	29.38	30		30.228	29.894	0.11	30.035925	30.248	0.1	30.26375	C_8	29.3	29.7		#VALUE!	0.356	-30.248	δ				ε							
	29.354	29.016	0.076	29.15159				10.2739	C_{10}	29.16	29.3		32.612	32.156	0.198	32.360645	32.569	0.1	32.6068	C_9	31.66	31.8		-3.258	-3.14	-32.569	γ				δε							
	27.851	27.533	0.045	27.6545375	$1-^{13}C$	28.028	0.01	27.968325	C_8	26.77	27.8		27.855	27.52	0.143	27.6697825			9.74925	C_7	26.77	27.8		-0.004	0.013	28.028	ε					0						
	ca 23			#VALUE!			#VALUE!	C_{17}	23	23.1		ca 14			#VALUE!			#VALUE!	C_{15}	14.22	14.5		#VALUE!	0	0	α					βγ							
	ca 23			#VALUE!			#VALUE!	C_2	22.97	23.1		ca 14			#VALUE!			#VALUE!	C_1	13.38	14.5		#VALUE!	0	0	α					βγ							
	ca 23			#VALUE!			#VALUE!	C_{12}	22.84	22.7		ca 14			#VALUE!			#VALUE!	C_{11}	14.1	14.1		#VALUE!	0	0	α					βγ							
	ca 14			#VALUE!			#VALUE!	C_{16}	14.3	14.1																				αβ							
	ca 14			#VALUE!			#VALUE!	C_{13}	14.29	14.1																				αβ							
	ca 14			#VALUE!			#VALUE!	C_1	14.17	14.2																				αβ							
C6-I	131.686	131.623	0.209	131.692598	$2-^{13}C$	132.041	-0.063	131.902418	C_{10}	131.8	130.6	C5-I	131.536	131.43	0.2	131.5126	131.812	0.01	131.717675	C_9	131.8	128		0.15	0.193	0.229	δ	C8-I	131.676	-0.01	ε							
	128.75	128.661	0.202	128.738105	$1-^{13}C$	129.043	-0.001	128.940223	C_8	130.51	128.6		128.977	128.869	0.188	128.94957	129.299	0.1	129.20905	C_8	130.51	128.7		-0.227	-0.208	-0.256	ε		128.696	-0.054		0						
	38.1	37.78		37.892	$2-^{13}C$	38.094	0.01	38.098375	C_7 (CH)	36.67	38.1		37.971	37.573	0.2	37.7578			13.28985	C_6 (CH)	36.67	37.8		0.129	0.207	38.094	δ		38.285	0.185	ε							
	37.066	36.648	0.251	36.8514025	$1-^{13}C$	37.24	-0.007	37.1775075	C_5	35.9	39.2		36.924	36.454	0.153	36.6533075			12.9234	C_7	35.9	39.2		0.142	0.194	37.24	ε		36.975	-0.091		0						
	ca 32.6			#REF!			#VALUE!	C_{11}	32.54	33.4		35.207	34.826	0.122	34.987105			12.32245	C_{10}	34.43	35.9		#VALUE!	-34.826	0	γ											
	ca 33.7	33.47		#REF!	$1-^{13}C$			#VALUE!	C_6	32.51	33.1		33.7	33.34	0.088	33.48602			11.795	C_5	32.51	33.1		#VALUE!	0.13	0	εε*						0					
	ca 34.4			#REF!			#VALUE!	C_{13}	32.51	32.8		36.718	36.206	0.172	36.42433	36.75	0.366	36.822065	C_{13}	32.27	35.9		#VALUE!	-36.206	-36.75	γ				δε							
	ca 32			#VALUE!			#VALUE!	C_3	32.48	31.8		ca 23			#VALUE!			#VALUE!	C_2	22.75	22.7		#VALUE!	0	0	β				γδ							
	ca 32			#VALUE!			#VALUE!	C_{12}	32.26	32.1		ca 23			#VALUE!			#VALUE!	C_{11}	22.93	23.3		#VALUE!	0	0	β				γδ							
	ca 29.8			#VALUE!			#VALUE!	C_5	29.85	29.6			32.37	31.956	0.142	32.133205			11.3295	C_3	32.2	32.1		#VALUE!	-31.956	0	γ				δε							
	ca 29			#VALUE!			#VALUE!	C_{16}	28.67	23.2		ca 20			#VALUE!			#VALUE!	C_{14}	20.38	20.6		#VALUE!	0	0	β				γδ							

	27.7154	27.37		27.49089	$2-^{13}C$			9.70039	C_5	27.29	27.6		27.745	27.346	0.175	27.5254625	27.819	0.1	27.81585	C_5	27.3	27.2		-0.0296	0.024	-27.819	δ				ε							
	ca 23			#VALUE!				#VALUE!	C_{17}	22.88	23		ca 14			#VALUE!			#VALUE!	C_{15}	14.17	14.4		#VALUE!	0	0	α				βγ							
	ca 23			#VALUE!				#VALUE!	C_9	22.83	22.7		ca 14			#VALUE!			#VALUE!	C_1	14.15	14.1		#VALUE!	0	0	α				βγ							
	ca 23			#VALUE!				#VALUE!	C_{13}	22.62	22.8		ca 14			#VALUE!			#VALUE!	C_{12}	13.55	14.2		#VALUE!	0	0	α				βγ							
	ca 14			#VALUE!				#VALUE!	C_{16}	14.13	14.1																			αβ							
	ca 14			#VALUE!				#VALUE!	C_1	14.05	14.1																			αβ							
	ca 14			#VALUE!				#VALUE!	C_{14}	13.9	14.2																			αβ							
																#REF!																					
C6-K	130.581	130.606	0.201	130.642978	$2-^{13}C$	130.978	-0.114	130.813115	C_{16}	131.36	130.6	C5-K	130.425	130.417	0.186	130.462115	130.736	-0.008	130.62533	C_5	132	128		0.156	0.189	0.242	δ	C8-K	130.585	0.004	ε							
	128.298	128.399	0.226	128.415065	$1-^{13}C$	128.692	0.006	128.555465	C_8	130.05	128.6		128.542	128.607	0.203	128.630433	128.859	0.193	128.791958	C_8	130.05	128.7		-0.244	-0.208	-0.167	ε		128.215	-0.083		0						
	38.437	38.085	0.22	38.25825	$2-^{13}C$	38.573	0.036	38.53359	C_7 (CH)	36.67	38.1		38.298	37.923	0.123	38.0822325	38.324	0.081	38.3333275	C_6 (CH)	36.67	37.8		0.139	0.162	0.249	δ		38.412	-0.025	ε							
	31.502	31.258	0.15	31.377525	$1-^{13}C$	31.722	-0.027	31.6388575	C_7	35.9	33.2		31.557	31.308	0.099	31.4176725	31.422	0.67	31.621675	C_7	35.9	33.2		-0.055	-0.05	0.3	ε		31.442	-0.06		0						
	33.97	33.614	0.155	33.7738625	$1-^{13}C$	34.092	0.038	34.057945	C_6	32.51	33.1		33.931	33.581	0.108	33.72807	33.97986	0.07423	33.9796463	C_6	32.51	33.1		0.039	0.033	0.11214	εε*		33.932	-0.038		0						
	33.646	33.245	0.522	33.504105		33.782	0.038	33.743045	C_{15}	32.51	32.8		36.389	36.043	0.126	36.192765	36.704	0.07	36.609675	C_{13}	32.27	35.9		-2.743	-2.798	-2.922	γ		33.917	0.271	δε							
	32.351	31.986	0.185	32.1558375				11.32285	C_5	32.48	31.8		23.08	22.764	0.089	22.8948475	23.134	0.1	23.13785	C_5	22.75	22.7		9.271	9.222	-23.134	β				γδ							
	30.364	30.073	0.344	30.25311				10.6274	C_{12}	31.63	32.1		21.236	20.932	0.09	21.058875			7.4326	C_{11}	22.7	23.3		9.128	9.141	0	β				γδ							
	30.164	29.79	0.164	29.95821		29.855	0.153	29.9979575	C_8	29.85	29.6		32.756	32.38	0.085	32.5309375	32.65	0.01	32.689375	C_8	32.2	32.1		-2.592	-2.59	-2.795	γ				δε							
	29.456	29.097	0.164	29.25996		29.535	0.054	29.519635	C_{16}	28.67	23.2		21.235	20.927	0.074	21.051635			7.43225	C_{14}	20.38	20.6		8.221	8.17	29.535	β				γδ							
	27.179	26.807	0.197	26.9820175	$2-^{13}C$	27.297	0.069	27.2713975	C_5	27.29	27.5		26.901	26.528	0.095	26.6801625	27.10344	-0.29479	26.9655213	C_5	27.3	27.2		0.278	0.279	0.19356	δ		27.153	-0.026	ε							
	27.409	27.114	0.139	27.2488725		27.584	0.008	27.52457	C_{11}	25.78	27.4		29.794	29.508	0.093	29.6292575	29.8525	0.019	29.8363475	C_{10}	29.5	29.9		-2.385	-2.394	-2.2685	γ		27.66	0.251	δε							
	ca 23			#VALUE!				#VALUE!	C_{17}	22.88	23		ca 14			#VALUE!			#VALUE!	C_{15}	14.17	14.4		#VALUE!	0	0	α				βγ							
	ca 23			#VALUE!				#VALUE!	C_9	22.83	22.7		ca 14			#VALUE!			#VALUE!	C_1	14.15	14.1		#VALUE!	0	0	α				βγ							
	ca 23			#VALUE!				#VALUE!	C_{13}	22.11	22.8		13.73	13.61	0.079	13.6699725			#REF!	C_{12}	13.8	14.2		#VALUE!	-13.61	0	α				βγ							
	ca 14			#VALUE!				#VALUE!	C_{16}	14.13	14.1																			αβ							
	ca 14			#VALUE!				#VALUE!	C_1	14.05	14.1																			αβ							
	ca 14			#VALUE!				#VALUE!	C_{14}	13.7	14.2																			αβ							
C6-L	135.165	*135.184*	*0.186*	135.219665	$1-^{13}C$	135.454	-0.08	135.33465	C_5	138.4	136.3	C5-L	135.347	135.234	0.1	135.2963			47.37145	C_5	138.4	136.4		-0.182	-0.05	135.454	εε*	C8-L					0						
	129.7	*129.464*	0.198	129.591645	$2-^{13}C$	129.963	-0.052	129.85912	C_5	124.6	129		129.562	129.276	0.261	129.435478			45.3467	C_4	124.6	129.8		0.138	0.188	129.963	δ				ε							
	37.475	*37.098*	0.23	37.282275	$2-^{13}C$	37.632	0.042	37.586605	C_7 (CH)	43.19	37.1		37.347	36.931	0.185	37.1186875	37.467	0.1	37.44775	C_6 (CH)	43.19	36.8		0.128	0.167	0.165	δ		37.485	0.01	ε							
	36.488	*35.992*	0.218	36.215195		36.311	0.126	36.401615	C_{15}	34.95	35.2		38.857	38.379	0.043	38.5560825	39.101	0.1	39.03835	C_{13}	34.95	33		-2.369	-2.387	-2.79	γ		36.645	0.157	δε							
	36.186	*35.69*	0.217	35.9129675	$1-^{13}C$	36.553	0.075	36.4416125	C_8	34.95	35.5		36.205	35.784	0.154	35.966385	36.21	0.1	36.231	C_7	34.95	35.5		-0.019	-0.094	0.343	ε		36.177	-0.009		0						
	30.228	*29.872*	0.293	30.0632575	$2-^{13}C$	30.383	0.01	30.331025	C_{10}	32.26	30		30.014	29.709	-0.036	29.80756	29.968	0.1	30.00685	C_9	29.51	29.7		0.214	0.163	0.415	δ				ε							
	32.403	*31.931*	*0.298*	32.163995		32.575	0.01	32.517075	C_3	31.95	32.1		23.227	22.91	0.132	23.05098			8.12945	C_2	22.98	23.3		9.176	9.021	32.575	β				γδ							
	32.532	*32.166*	0.201	32.3398275		32.376	0.01	32.432875	C_{12}	31.86	31.9		23.41	23.012	0.275	23.2138625			8.1935	C_{11}	22.74	22.7		9.122	9.154	32.376	β				γδ							
	29.975	*29.615*	0.179	29.7817225		30.104	0.01	30.061125	C_{16}	29.53	29.7		20.819	20.484	0.151	20.6356025			7.28665	C_{14}	20	20.6		9.156	9.131	30.104	β				γδ							
	29.794	*29.373*	0.204	29.56676		29.874	0.01	29.848275	C_{11}	29.16	29.3		32.334	31.909	0.146	32.090965			11.3169	C_{10}	31.94	31.8		-2.54	-2.536	29.874	γ				δε							
	27.781	*27.45*	0.197	27.6106675		27.942	0.015	27.8890625	C_8	27.47	27.7		30.54	30.154	-0.159	30.2529275			10.689	C_3	29.43	30.2		-2.759	-2.704	27.942	γ				δε							
	27.77	*27.39*	0.219	27.5728225	$1-^{13}C$	27.926	0.039	27.8802725	C_5	28.32	27.5		27.852	27.5	0.261	27.6825775	28.058	0.1	28.00865	C_5	28.32	27.5		-0.082	-0.11	-0.132	ε						0					
	23.298	*22.933*	*0.244*	23.11626		23.397	0.01	23.364625	C_{17}	23.06	23.1		ca 14			#VALUE!			#VALUE!	C_{15}	14.1	14.5	na		22.933	23.397	α				βγ							
	23.09	*22.694*	*0.245*	22.8883375		23.126	0.01	23.115675	C_{13}	22.84	22.7		ca 14			#VALUE!			#VALUE!	C_{12}	14.1	14.1	na		22.694	23.126	α				βγ							
	22.765	*22.438*	*0.238*	22.606595		22.816	0.01	22.800425	C_2	22.3	22.8		ca 14			#VALUE!			#VALUE!	C_1	13.85	14.2	na		22.438	22.816	α				βγ							
	14.266	*14.133*	*0.069*	14.1952475		14.394	0.01	14.351475	C_{14}	14.25	14.1																			αβ							
	14.257	*14.117*	*0.071*	14.1821525		14.351	0.01	14.320375	C_{18}	14	14.1																			αβ							
	14.172	*14.024*	*0.074*	14.092635		14.235	0.01	14.215225	C_1	13.9	14.2																			αβ							
C6-M	135.263	*135.112*	0.198	135.209895	$1-^{13}C$	135.517	-0.036	135.41991	C_5	133.75	136.3	C5-M	135.479	135.296	0.157	135.395768			47.41765	C_5	133.75	136.4		-0.216	-0.184	135.517	εε*	C8-M	135.232	-0.031			0						
	130.22	*129.934*	0.25	130.090975	$2-^{13}C$	130.495	-0.048	130.38783	C_5	127.7	129		130.09	129.759	0.188	129.91762			45.5315	C_4	127.7	129.8		0.13	0.175	130.495	δ				ε							
	43.28	*42.768*	0.262	43.006805	$2-^{13}C$	43.426	0.027	43.3810425	C_7 (CH)	43.19	43.1		43.14	42.574	0.251	42.8292025	43.029	0.1	43.0906	C_6 (CH)	43.19	42.8		0.14	0.194	0.397	δ		43.272	-0.008	ε							
	36.024	*35.583*	0.292	35.80378	$1-^{13}C$	36.162	-0.072	36.09732	C_8	34.95	35.5		38.397	37.885	0.215	38.1131125			13.43895	C_{13}	34.95	33		-2.373	-2.302	36.162	γ		36.043	0.019		0						
	35.754	*35.285*	0.239	35.5035225		35.851	0.067	35.8322925	C_{15}	34.95	35.2		36.11	35.619	0.159	35.8270225	36.06	0.1	36.10025	C_7	34.95	35.5		-0.356	-0.334	-0.209	ε				δε							
	32.673	*32.291*	0.292	32.49113		32.78	0.01	32.744825	C_3	32.75	33.7		32.432	32.112	0.072	32.24038	32.416	0.1	32.44435	C_8	29.51	29.7		0.241	0.179	0.364	δ				δε							
	30.189	*29.755*	0.206	29.953765	$2-^{13}C$	30.276	0.131	30.2753525	C_{10}	32.26	30		21.134	20.822	0.107	20.9555425			7.3969	C_9	22.71	23.3		9.055	8.933	30.276	β				ε							
	32.367	*31.919*	0.309	32.1460975		32.384	0.01	32.380325	C_3	32.17	32.1		23.227	22.91	0.132	23.05098	23.28	0.1	23.2842	C_{11}	22.74	22.7		9.14	9.009	9.104	β				γδ							
	32.375	*31.953*	*0.293*	32.1673575		32.354	0.01	32.363625	C_{12}	31.86	31.9		23.198	22.876	0.132	23.01873	23.21	0.1	23.22855	C_{14}	20	20.6		9.177	9.077	9.144	β				γδ							
	29.984	*29.534*	0.229	29.7435975		30.014	0.01	30.005775	C_{16}	29.53	29.7		32.755	32.34	-0.029	32.4786525	32.652	0.1	32.7108	C_{10}	31.94	31.8		-2.771	-2.806	-2.638	γ				γδ							
	29.776	*29.362*	0.205	29.5535375		29.865	0.01	29.836125	C_{11}	29.16	29.3		32.373	31.949	0.146	32.130615	32.229	0.1	32.30215	C_9	34.33	36.2		-2.597	-2.587	-2.364	γ				δε							
	27.656	*27.271*	0.218	27.455345	$1-^{13}C$	27.849	-0.036	27.77326	C_8	28.32	27.5		27.655	27.251	0.174	27.431985	27.761	0.1	27.74665	C_8	28.32	27.5		0.001	0.02	0.088	ε						0					
	23.192	*22.835*	*0.245*	23.0156875		23.299	0.01	23.263825	C_{17}	23.06	23.1		ca 14			#VALUE!			#VALUE!	C_{15}	14.1	14.5	na		22.835	23.299	α				βγ							
	23.09	*22.694*	*0.245*	22.8883375		23.126	0.01	23.115675	C_{13}	22.84	22.7		ca 14			#VALUE!			#VALUE!	C_{12}	14.1	14.1	na		22.694	23.126	α				βγ							
	22.501	*22.138*	*0.255*	22.3230625		22.555	0.01	22.538375	C_2	22.1	22.8		13.754	13.656	0.078	13.708045			4.8139	C_1	13.72	14.2	na	na		22.555	α				βγ							
	14.271	*14.143*	*0.07*	14.203725		14.412	0.01	14.364925	C_{14}	14.25	14.1																			αβ							
	14.264	*14.121*	*0.074*	14.187885		14.356	0.01	14.326075	C_{18}	14	14.1																			αβ							
	14.081	*13.952*	*0.071*	14.0133025		14.156	0.01	14.132025	C_1	13.8	14.2																			αβ							

synthetic:

neat shift difference to "trimer"

C6-L	135.186	135.184	0.186	135.227015	C_5	138.4	136.3	0.021
	129.747	129.464	0.237	129.616968	C_5	124.6	129	0.047
	37.537	37.098	0.308	37.32172	C_7	43.19	37.1	0.062
	36.554	35.992	0.312	36.25968	C_{15}	34.95	35.2	0.066
	36.251	35.69	0.313	35.9575575	C_8	34.95	35.5	0.065
	30.337	29.872	0.291	30.1009525	C_{10}	32.26	30	0.109
	32.403	31.931	0.298	32.163995	C_3	31.95	32.1	0
	32.579	32.166	0.271	32.3722025	C_{12}	31.86	31.9	0.047
	30.037	29.615	0.29	29.828675	C_{16}	29.53	29.7	0.062
	29.864	29.373	0.29	29.610825	C_{11}	29.16	29.3	0.07
	27.828	27.45	0.26	27.64145	C_8	27.47	27.7	0.047
	27.838	27.39	0.298	27.614595	C_8	28.32	27.5	0.068
	23.298	22.933	0.244	23.11626	C_{17}	23.06	23.1	0
	23.09	22.694	0.245	22.8883375	C_{13}	22.84	22.7	0
	22.765	22.438	0.238	22.606595	C_2	22.3	22.8	0
	14.266	14.133	0.069	14.1952475	C_{14}	14.25	14.1	0
	14.257	14.117	0.071	14.1821525	C_{18}	14	14.1	0
	14.172	14.024	0.074	14.092635	C_1	13.9	14.2	0
								0
C6-M	135.291	135.112	0.215	135.223563	C_5	133.75	136.3	0.028
	130.283	129.934	0.291	130.122353	C_5	127.7	129	0.063
	43.346	42.768	0.37	43.054475	C_7	43.19	43.1	0.066
	36.114	35.583	0.319	35.8414225	C_8	34.95	35.5	0.09
	35.815	35.285	0.319	35.5430725	C_{15}	34.95	35.2	0.061
	32.703	32.291	0.27	32.496625	C_8	32.75	33.7	0.03
	30.208	29.755	0.292	29.97998	C_{10}	32.26	30	0.019

32.350	31.919	0.250	32.15098
32.375	31.953	0.253	32.1673575
29.965	29.534	0.256	29.75219
29.847	29.362	0.291	29.5979525
27.724	27.271	0.298	27.497345
23.182	22.835	0.245	23.0156875
23.09	22.694	0.245	22.8883375
22.501	22.138	0.256	22.3230625
14.271	14.143	0.07	14.203725
14.264	14.121	0.074	14.187885
14.081	13.952	0.071	14.0133025

C_1	32.17	32.1	0.025
C_{12}	31.86	31.9	0
C_{18}	29.53	29.7	-0.019
C_{11}	29.16	29.3	0.071
C_6	28.32	27.5	0.068
C_{17}	23.06	23.1	0
C_{13}	22.84	22.7	0
C_5	22.1	22.8	0
C_{14}	14.25	14.1	0
C_{16}	14	14.1	0
C_{15}	13.8	14.2	0